Modeling Elasticity in Crystal Growth

Ken Elder, Oakland University, DMR Award #0076054

The appearance and growth of crystal phases occurs in many technologically important processes including semiconductor device fabrication (e.g., epitaxial growth) and metal purification (e.g., zone refinement). The microstructures created by these non-equilibrium processes strongly influence material properties such as hardness, reactivity, and failure rates in electronic devices. Unfortunately it has proven difficult to model such phenomena due to the influence of long-range elastic forces and the singular nature of crystal imperfections or defects.

To overcome these difficulties a new model was developed by the PI and collaborators. This model treats elastic forces and crystal defects exactly and leads to simulations that are orders magnitude faster than conventional atomic simulations. For example, this new model can simulate the solidification of copper at 650°C approximately one billion times faster than molecular dynamics simulations.

Grain Growth

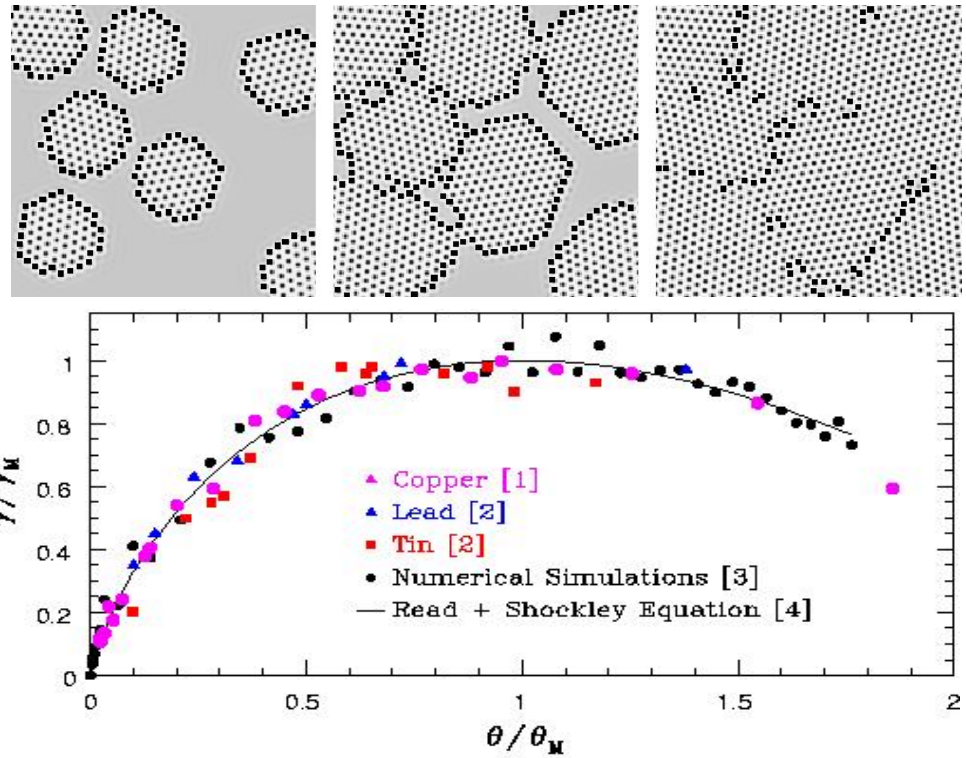

Figure 1. Grain Growth: In the upper figure simulation data for the crystallization of a supercooled melt [3] is shown at three consecutive times. In the bottom figure the grain boundary energy predicted by Elder *et. al.* [3] is compared with experimental and theoretical results.

[1] Gjostein + Rhines, Acta. Metall. **7**, 319 (1959), [2] Aust+Chalmers, Metal Interfaces (American Society of Metals, Cleveland, Ohio, 1952). [3] Elder *et. al.* , PRL **88**, 245701 (2002). [4] Read + Shockley **78**, 275 (1950).

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Numerical simulations of the new model were shown to be consistent with grain boundary energy measurements (Fig. 1) and provided the first realistic simulations of grain growth on diffusive time scales. In addition, simulations of epitaxial growth were consistent with critical thickness measurements (Fig. 2) and predicted the surface roughening behavior observed in very recent measurements on SiGe/Si heterostructures.

Collaborators

Undergraduate, M. Katakowski, Oakland U.
Graduate, M. Haataja, McGill U.
Faculty, M. Grant, McGill U.

Invited presentations ;

NIST, Gaithersburg, May 10 2001
LANL, Los Alamos, May 16 2001
McGill U., Montreal, Dec. 7 2001
Helsinki U. of Tech, Helsinki, Feb. 4 2002
TMS annual meeting, Seattle, Feb. 19 2002

Publications;

Elder, Katakowski, Haataja, and Grant, Phys. Rev. Lett., **88**, 245701 (2002)

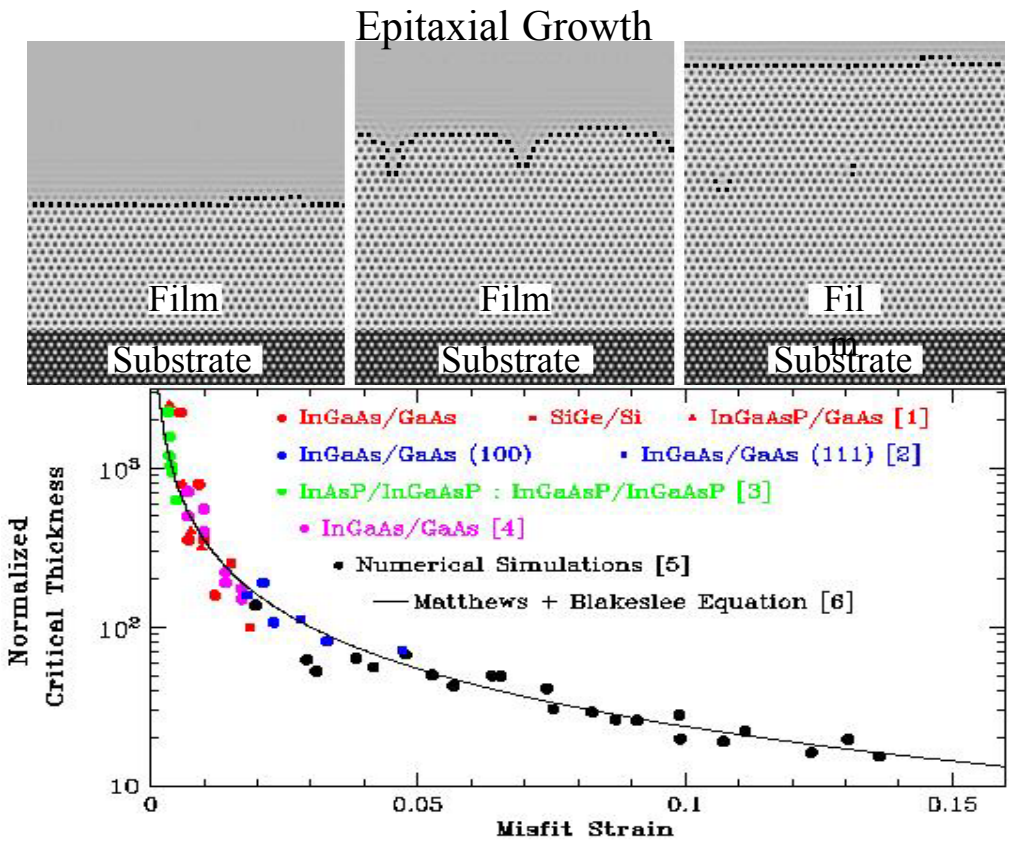

Figure 2. Epitaxial Growth: In the upper figure numerical simulations [5] of heteroepitaxial growth are shown at three consecutive times. In the lower figure the critical thickness at which defects nucleate is compared with experimental and theoretical results. [1] Bolkhovityanov et.al. J.AP **73**, 15 (1996). [2] Anan, Nishi + Suguo, APL **60**, 22 (1992). [3] Ogasawara, JAP **84**, 4775 (1998). [4] Rocket + Kelly, PRB **44**, 1154 (1991). [5] Elder et. al. PRL **88**, 245701 (2002) . [6] Matthews + Blakeslee, J. Cryst. **27**, 118 (1974).